

Endothal
145-73-3 | DTXSID7024081

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.93

Global applicability domain: Outside

Local applicability domain index: 4.01e-01

Confidence level: 8.20e-01

Nearest Neighbors from the Training Set

Image not found

2,5-Pyridinedicarboxylic acid

Measured: 5.75

Predicted: 4.09